Supporting Information

Potentiation of *Francisella* Resistance to Conventional Antibiotics through Small Molecule Adjuvants

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Initial pilot screen. 1-5

SI Figure 1 Compounds from initial pilot screen.

MIC Results of SAR study.

SI Table 1 MIC results of SAR study.

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**Synthetic procedures and compound characterization**

\textit{N-(2-(1H-indol-3-yl)ethyl)-4-butylbenzamide (5).} White solid; yield 93%: \textit{1H NMR} (300 MHz, CDCl\textsubscript{3}), \( \delta \) 8.43 (br, 1H), 7.66-7.59 (m, 3H), 7.37 (d, \( J = 8.1 \) Hz, 1H), 7.24-7.10 (m, 4H), 7.03 (s, 1H), 6.32 (br, 1H), 3.79 (q, \( J = 6 \) Hz, 2H), 3.08 (t, \( J = 6.6 \) Hz, 2H), 2.62 (t, \( J = 7.2 \) Hz, 2H), 1.58 (q, \( J = 8.1 \) Hz, 2H), 1.34 (sext, \( J = 7.2 \) Hz, 2H), 0.93 (t, \( J = 7.2 \) Hz, 3H); \textit{13C NMR} (100 MHz, CDCl\textsubscript{3}), \( \delta \) 168.0, 147.1, 136.9, 132.4, 129.0, 127.7, 127.3, 122.7, 122.6, 119.8, 119.1, 113.3, 111.8, 40.7, 35.9, 33.8, 25.7, 22.7, 14.3; HRMS (ESI) calcd. for C\textsubscript{21}H\textsubscript{22}N\textsubscript{2}O [M+H]\textsuperscript{+}: 321.19614, found: 321.19576.
4-butyl-N-phenethylbenzamide (9). White solid; yield 93%; $^1$H NMR (300 MHz, CDCl$_3$), δ 7.60 (d, $J = 8.1$ Hz, 2H), 7.35-7.31 (m, 2H), 7.26-7.19 (m, 5H), 6.14 (br, 1H), 3.71 (q, $J = 6.6$ Hz, 2H), 2.93 (t, $J = 6.9$ Hz, 2H), 2.63 (t, $J = 7.5$ Hz, 2H), 1.64-1.54 (m, 2H), 1.34 (sext, $J = 7.2$ Hz, 2H), 0.92 (t, $J = 7.5$ Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$), δ 167.7, 147.0, 139.2, 132.2, 129.1, 128.9, 128.8, 127.0, 126.8, 41.3, 36.0, 35.7, 33.6, 22.5, 14.1; HRMS (ESI) calcd. for C$_{19}$H$_{23}$NO [M+H]$^+$: 282.18524, found: 282.18477.

$\text{N-(2-(1H-indol-3-yl)ethyl)-4-methylbenzamide (8).}$ White solid; yield 55%; $^1$H NMR (300 MHz, CDCl$_3$), δ 8.36 (br, 1H), 7.65-7.57 (m, 3H), 7.38 (d, $J = 7.8$ Hz, 1H), 7.24-7.10 (m, 4H), 7.04 (s, 1H), 6.32 (br, 1H), 3.79 (q, $J = 6.3$ Hz, 2H), 3.09 (t, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$), δ 167.7, 141.9, 136.6, 131.8, 129.3, 127.4, 127.2, 127.0, 122.3, 122.2, 119.5, 118.8, 113.0, 111.5, 40.4, 25.4, 21.5; HRMS (ESI) calcd. for C$_{18}$H$_{18}$N$_2$O [M+H]$^+$: 279.14914, found: 279.14879.

$\text{N-(2-(1H-indol-3-yl)ethyl)-4-ethylbenzamide (7).}$ Tan solid; yield 90%; $^1$H NMR (300 MHz, CDCl$_3$), δ 8.22 (br, 1H), 7.67-7.59 (m, 3H), 7.38 (d, $J = 8.4$ Hz, 1H), 7.24-7.11 (m, 4H), 7.06 (s, 1H), 6.25 (br, 1H), 3.80 (q, $J = 6.6$ Hz, 2H), 3.09 (t, $J = 6.6$ Hz, 2H), 2.66 (q, $J = 6.3$ Hz, 2H), 1.23 (t, $J = 7.2$ Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$), δ 167.7, 148.1, 136.6, 132.1, 128.9, 127.6, 127.1, 122.3, 119.5, 118.8, 115.4, 112.9, 111.5, 40.4, 25.4, 15.4; HRMS (ESI) calcd. for C$_{19}$H$_{20}$N$_2$O [M+H]$^+$: 293.16484, found: 293.16430.

$\text{N-(2-(1H-indol-3-yl)ethyl)-4-propylbenzamide (6).}$ White solid; yield 89%; $^1$H NMR (300 MHz, CDCl$_3$), δ 8.12 (br, 1H), 7.66 (d, $J = 6.9$ Hz, 1H), 7.59 (d, $J = 7.8$ Hz, 2H), 7.39 (d, $J = 8.4$ Hz, 1H), 7.25-7.11 (m, 4H), 7.08 (s, 1H), 6.21 (br, 1H), 3.80 (q, $J = 6.3$ Hz, 2H), 3.09 (t, $J = 6.6$ Hz, 2H), 2.60 (t, $J = 7.2$ Hz, 2H), 1.63 (q, $J = 7.2$ Hz, 2H), 0.92 (t, $J = 7.5$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$), δ 167.9, 146.7, 136.7, 132.3, 128.9, 127.6, 127.1, 122.5, 122.4, 119.7, 119.0, 113.1, 111.6, 40.5, 38.1, 25.6, 24.6, 14.0; HRMS (ESI) calcd. for C$_{20}$H$_{22}$N$_2$O [M+H]$^+$: 307.17997.

$\text{N-(2-(1H-indol-3-yl)ethyl)-4-methoxybenzamide (15).}$ White solid; yield 79%; $^1$H NMR (300 MHz, CDCl$_3$), δ 8.32 (br, 1H), 7.64 (d, $J = 8.7$ Hz, 3H), 7.38 (d, $J = 8.1$ Hz, 1H), 7.24-7.09 (m, 3H), 7.04 (s, 1H), 6.86 (d, $J = 6.0$ Hz, 2H), 6.27 (br, 1H), 3.82-3.75 (m, 5H), 3.08 (t, $J = 6.6$ Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$), δ 167.2, 162.2, 136.6, 128.8, 127.4, 126.9, 122.3, 119.6, 118.9, 113.8, 113.1, 111.5, 55.5, 40.4, 25.5; HRMS (ESI) calcd. for C$_{19}$H$_{18}$N$_2$O$_2$ [M+H]$^+$: 295.14410, found: 295.14353.
**N-(2-(1H-indol-3-yl)ethyl)-4-butylbenzenesulfonamide (12).** White solid; yield 92%; ^1H NMR (300 MHz, CDCl$_3$), δ 8.12 (br, 1H), 7.66 (d, $J$ = 8.4 Hz, 2H), 7.42 (d, $J$ = 7.5 Hz, 1H), 7.35 (d, $J$ = 7.7 Hz, 1H), 7.24-7.16 (m, 3H), 7.09-7.03 (m, 1H), 6.96 (s, 1H), 5.28-3.27 (m, 2H), 2.93 (t, $J$ = 6.3 Hz, 2H), 2.65 (t, $J$ = 7.5 Hz, 2H), 1.65-1.55 (m, 2H), 1.41-1.31 (m, 2H), 0.94 (t, $J$ = 7.2 Hz, 3H); ^13C NMR (100 MHz, CDCl$_3$), δ 148.4, 137.0, 136.5, 129.1, 127.1, 127.0, 122.8, 122.3, 119.6, 118.6, 111.6, 111.5, 43.2, 35.6, 33.3, 25.6, 22.4, 14.0; HRMS (ESI) calcd. for C$_{20}$H$_{24}$N$_2$O$_2$S [M+H]$^+$: 357.16313, found: 357.16223.

**2-(1H-indol-3-yl)ethyl 4-butylbenzoate (11).** Yellow solid; yield 62%; ^1H NMR (300 MHz, CDCl$_3$), δ 8.05 (br, 1H), 7.97 (d, $J$ = 7.5 Hz, 2H), 7.70 (d, $J$ = 7.5 Hz, 1H), 7.38 (d, $J$ = 8.1 Hz, 1H), 7.26-7.10 (m, 5H), 4.60 (t, $J$ = 6.9 Hz, 2H), 3.25 (t, $J$ = 7.2 Hz, 2H), 2.67 (t, $J$ = 8.1 Hz, 2H), 1.62 (quin, $J$ = 7.8 Hz, 2H), 1.36 (sext, $J$ = 6.3 Hz, 2H), 0.94 (t, $J$ = 7.2 Hz, 3H); ^13C NMR (100 MHz, CDCl$_3$), δ 167.0, 148.7, 136.4, 129.9, 128.7, 128.1, 127.7, 122.4, 122.3, 119.7, 119.1, 112.4, 111.4, 65.1, 36.0, 33.5, 25.2, 22.6, 14.2; HRMS (ESI) calcd. for C$_{21}$H$_{23}$NO$_2$ [M+Na]$^+$: 344.16210, found: 344.16145.

**S-ethyl indoline-1-carbothioate (2).** Colorless oil; yield 95%; ^1H NMR (300 MHz, CDCl$_3$), δ 8.03 (d, $J$ = 7.8 Hz, 1H), 7.21-7.14 (m, 2H), 7.01-6.96 (m, 1H), 3.99 (t, $J$ = 9.0 Hz, 2H), 3.16 (t, $J$ = 8.1 Hz, 2H), 2.99 (q, $J$ = 7.2 Hz, 2H), 1.35 (t, $J$ = 7.2 Hz, 3H); ^13C NMR (100 MHz, CDCl$_3$), δ 165.7, 142.9, 131.1, 127.6, 124.8, 123.6, 115.9, 47.3, 27.9, 24.6, 15.4; HRMS (ESI) calcd. for C$_{11}$H$_{13}$NOS [M+H]$^+$: 208.07906, found: 208.07872.

**SI Scheme 1.** Synthetic scheme for the synthesis of amine 10.

**N-(4-butylbenzyl)-2-(1H-indol-3-yl)ethan-1-amine (10).** In a flame dried round bottom under N$_2$ atmosphere was added amide 5 (200.0 mg, 0.62 mmol) and anhydrous THF (10 mL). The reaction mixture was cooled to 0°C and LAH (3.12 mL, 6.24 mmol) was added dropwise. The reaction was allowed to warm to rt before being heated to reflux. After the reaction was complete the reaction was cooled to 0°C and slowly quenched with H$_2$O. After quenching, a sat. solution of Rochelle’s salt was added and the mixture was stirred until two visible layers were observed. The aq. layer was extracted with EtOAc (3 x 10 mL) and the combined organic layers were washed with brine (1 x 10 mL) and dried over Na$_2$SO$_4$, then filtered. The solvent was removed in vacuo and the residue was purified by flash chromatography using DCM/2% MeOH/2% TEA to deliver product as a yellow oil (130.1 mg, 68%). ^1H NMR (300 MHz, CDCl$_3$), δ 8.09 (br, 1H), 7.61 (d, $J$ = 7.8 Hz, 1H), 7.35 (d, $J$ = 7.5 Hz, 1H), 7.22-7.17 (m, 3H), 7.13-7.09 (m, 3H), 7.02 (s, 1H), 3.79 (s, 2H), 3.06 (s, 3H) 2.58 (t, $J$ = 7.2 Hz, 2H), 1.63-1.53 (m, 2H), 1.40-1.31 (m, 2H), 1.23-1.18 (m, 2H), 0.92 (t, $J$ = 7.5 Hz, 3H); ^13C NMR (100 MHz, CDCl$_3$), δ 165.7, 137.2, 136.5, 128.6, 128.3, 127.6, 124.8, 123.6, 115.9, 47.3, 27.9, 24.6, 15.4; HRMS (ESI) calcd. for C$_{21}$H$_{26}$N$_2$ [M+H]$^+$: 307.21688, found: 307.21658.

**SI Scheme 2.** Synthetic scheme for the synthesis of tryptamines derivatives 16 and 17.
General procedure for indole alkylation or acylation:
In a flame dried round bottom under N\textsubscript{2} atmosphere was added tryptamine (300 mg, 1.87 mmol) and anhydrous DMF (10 mL). The reaction mixture was cooled to 0°C and NaH (82.4 mg, 2.06 mmol) was added in a single portion. The reaction was stirred for 30 min before MeI (128 μL, 2.06 mmol) was added dropwise. After completion the reaction was poured into H\textsubscript{2}O and extracted with EtOAc (3 x 5 mL). The combined organic layers were washed with brine (1 x 5 mL) and dried over Na\textsubscript{2}SO\textsubscript{4}, then filtered. The solvent was removed in vacuo and the resulting residue was purified by flash chromatography using DCM/2% MeOH/2% TEA to afford pure product as a yellow oil (176.0 mg, 54%).

2-(1-methyl-1\textsubscript{H}-indol-3-yl)ethan-1-amine (16). Yellow Oil; yield 54%; \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}), δ 7.64-7.60 (m, 1H), 7.32-7.21 (m, 2H), 7.14-7.09 (m, 1H), 6.90 (s, 1H), 3.75 (s, 3H), 3.04-3.00 (m, 2H), 2.96-2.89 (m, 2H), 1.90 (s, 2H); \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}), δ 137.2, 128.0, 127.0, 121.7, 119.1, 118.8, 112.0, 109.3, 42.5, 32.7, 29.2; HRMS (ESI) calcd. for C\textsubscript{11}H\textsubscript{14}N\textsubscript{2} [M+H]\textsuperscript{+}: 175.12298, found: 175.12294.

1-(3-(2-aminoethyl)-1\textsubscript{H}-indol-1-yl)ethan-1-one (17). Orange oil; yield 60%; \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}), δ 7.59 (d, J = 6 Hz, 1H), 7.38-7.36 (m, 1H), 7.21-7.17 (m, 1H), 7.02 (s, 1H), 3.61-3.55 (m, 2H), 2.98-2.92 (m, 2H), 2.58 (s, 3H), 1.91 (s, 2H); \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}), δ 170.3, 136.5, 127.4, 122.3, 122.2, 119.4, 118.7, 118.7, 111.5, 39.9, 25.4, 23.5; HRMS (ESI) calcd. for C\textsubscript{12}H\textsubscript{14}N\textsubscript{2}O [M+H]\textsuperscript{+}: 203.11789, found: 203.11755.

4-butyl-N-(2-(1-methyl-1\textsubscript{H}-indol-3-yl)ethyl)benzamide (13). White solid; yield 91%; \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}), δ 7.66-7.59 (m, 3H), 7.34-7.10 (m, 5H), 6.92 (s, 1H), 6.27 (br, 1H), 3.81-3.75 (m, 5H), 3.08 (t, J = 6.6 Hz, 2H), 2.63 (t, J = 7.5 Hz, 2H), 1.59 (quin, J = 7.5 Hz, 2H), 1.41-1.28 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H); \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}), δ 167.8, 147.0, 137.6, 132.5, 128.9, 128.2, 127.3, 122.2, 119.4, 119.3, 112.0, 109.8, 40.9, 35.9, 33.8, 33.1, 25.7, 22.7, 14.3; HRMS (ESI) calcd. for C\textsubscript{22}H\textsubscript{26}N\textsubscript{2}O [M+H]\textsuperscript{+}: 335.21179, found: 335.21105.

N-(2-(1-acetyl-1\textsubscript{H}-indol-3-yl)ethyl)-4-butylbenzamide (14). Yellow solid; yield 70%; \textsuperscript{1}H NMR (300 MHz, CDCl\textsubscript{3}), δ 8.05 (br, 1H), 7.36-7.30 (m, 4H), 7.17-7.12 (m, 3H), 7.02-6.97 (m, 2H), 4.10-4.05 (m, 2H), 3.06 (t, J = 8.4 Hz, 2H), 2.64 (t, J = 7.8 Hz, 2H), 2.19 (s, 3H), 1.65-1.56 (m, 2H), 1.36 (sext, J = 7.5 Hz, 2H), 0.95 (t, J = 6.0 Hz, 3H); \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}), δ 174.8, 173.7, 148.1, 136.3, 132.8, 128.8, 128.6, 127.5, 127.2, 122.1, 119.5, 118.8, 112.5, 111.2, 47.3, 35.7, 33.4, 26.3, 25.0, 22.4, 14.0; HRMS (ESI) calcd. for C\textsubscript{23}H\textsubscript{28}N\textsubscript{2}O\textsubscript{2} [M+H]\textsuperscript{+}: 363.20670, found: 363.20564.

3-(1H-indol-3-yl)propan-1-ol (18). 3-indolepropionic acid (1.00 g, 5.29 mmol) was dissolved in THF (20 mL) and cooled to 0°C before dropwise addition of BH$_3$·THF (22.0 mL, 21.76 mmol). The reaction was allowed to warm to rt and stir for 48 hr. The reaction was quenched at 0°C with EtOH and was poured into H$_2$O (40 mL) and EtOAc (40 mL). A cloudy emulsion formed and sat. NaHCO$_3$ (20 mL) was added. The layers were separated and the organic layer was washed with brine (1 x 40 mL) and dried over Na$_2$SO$_4$, then filtered. The solvent was removed in vacuo and the residue was purified by flash chromatography using 1:1 Hex/EtOAc to afford the product as a yellow oil (627.3 mg, 68% yield).

$^1$H NMR (300 MHz, CDCl$_3$), δ 8.04 (br, 1H), 7.62 (d, $J$ = 8.1 Hz, 1H), 7.36 (d, $J$ = 8.4 Hz, 1H), 7.22-7.09 (m, 2H), 7.00 (s, 1H), 3.74 (t, $J$ = 6.3 Hz, 2H), 2.97 (s, 1H), 2.90-2.84 (m, 2H), 2.00 (quin, $J$ = 6.3 Hz, 2H);

$^{13}$C NMR (100 MHz, CDCl$_3$), δ 136.5, 127.6, 122.1, 121.4, 119.3, 119.0, 116.1, 111.2, 62.8, 33.0, 21.5; HRMS (ESI) calcd. for C$_{11}$H$_{13}$NO [M+H]$^+$: 176.10699, found: 176.10695.

3-(3-azidopropyl)-1H-indole (19). In a flame dried round bottom under N$_2$ atmosphere was added alcohol 18 (620.0 mg, 3.54 mmol), TEA (1.0 mL, 7.08 mmol), and anhydrous DCM (10 mL). The reaction mixture was cooled to 0°C, MsCl (301 μL, 3.89 mmol) was added dropwise and allowed to warm to rt for 3 hr. The reaction was washed with brine (1 x 5 mL), and dried over Na$_2$SO$_4$, then filtered. The solvent was removed in vacuo and the residue was dissolved in anhydrous DMF (10 mL) and NaN$_3$ (460.0 mg, 7.08 mmol) was added in a single portion. The reaction was heated to 60°C and allowed to stir overnight. After completion the reaction was cooled to rt and poured into H$_2$O and extracted with EtOAc (3 x 10 mL). The combined organics were washed with brine (1 x 10 mL) and dried over Na$_2$SO$_4$, then filtered. The solvent was removed in vacuo and the residue was purified by flash chromatography using 8:1 Hex/EtOAc to give the product as a yellow oil (490.0 mg, 69% yield).

$^1$H NMR (300 MHz, CDCl$_3$), δ 7.95 (br, 1H), 7.62 (d, $J$ = 7.2 Hz, 1H), 7.39-7.36 (m, 1H), 7.25-7.12 (m, 2H), 7.01 (s, 1H), 3.34 (t, $J$ = 6.9 Hz, 2H), 2.89 (t, 7.2 Hz, 2H), 2.02 (quin, $J$ = 6.9 Hz, 2H);

$^{13}$C NMR (100 MHz, CDCl$_3$), δ 136.6, 127.6, 122.3, 121.8, 119.6, 119.1, 115.3, 111.4, 51.3, 29.5, 22.4.

3-(1H-indol-3-yl)propan-1-amine (20). The azide 19 (470.0 mg, 2.35 mmol) was dissolved in THF (10 mL) and 10% Pd/C (100.0 mg) was added. The atmosphere was removed under vacuum and back filled with a H$_2$ balloon. The reaction was stirred overnight and then filtered through a pad of celite. The solvent was removed in vacuo and the residue was used directly in the next step.

N-(3-(1H-indol-3-yl)propyl)-4-butylbenzamide (4). White solid; yield 45%; $^1$H NMR (300 MHz, CDCl$_3$), δ 8.19 (br, 1H), 7.61 (d, $J$ = 7.2 Hz, 1H), 7.48 (d, $J$ = 8.1 Hz, 2H), 7.35 (d, $J$ = 8.1 Hz, 1H), 7.26-7.09 (m, 4H), 7.00 (s, 1H), 6.19 (br, 1H), 3.54-3.52 (m, 2H), 2.90-2.85 (m, 2H), 2.65-2.60 (m, 2H), 2.04 (quin, $J$ = 6.6 Hz, 2H), 1.59 (quin, $J$ = 6.3 Hz, 2H), 1.40-1.31 (m, 2H), 0.94 (t, $J$ = 6.0 Hz); $^{13}$C NMR (100 MHz, CDCl$_3$), δ 168.0, 147.1, 136.9, 132.3, 128.9, 127.6, 127.2, 122.4, 122.1, 119.7, 119.2, 115.8, 111.7, 40.4, 35.9, 33.8, 30.1, 23.3, 22.7, 14.4; HRMS (ESI) calcd. for C$_{22}$H$_{26}$N$_2$O [M+H]$^+$: 335.21179, found: 335.21103.

SI Scheme 4. Synthetic scheme for the synthesis of amine 1.

5,6-dimethyl-1H-benzo[d]imidazol-2-amine (1). 4,5-dimethylbenzene-1,2-diamine (1.00 g, 7.34 mmol) was dissolved in H$_2$O (100 mL) and MeOH (100 mL). BrCN (3.11 g, 29.36 mmol) was added in a single portion and the reaction was heated to reflux. After cooling the solvent was removed in vacuo and basified with 1M NaOH (40 mL). The aq. layer was extracted with EtOAc (3 x 30 mL). The organic layer was washed with brine and dried over Na$_2$SO$_4$, then filtered. The solvent was removed and the solid was dissolved in MeOH (10 mL) and acidified with conc. HCl. The solvent was removed a final time to give a brown solid (1.21 g, 83% yield). $^1$H NMR (300 MHz, DMSO-$d_6$), δ 8.45 (s, 2H), 7.12 (s,
2-(4-pentylphenyl)-4,5-dihydroxazole (3). 2-Bromoethylamine hydrobromide (265.2 mg, 1.29 mmol) was dissolved in anhydrous toluene (7 mL) in a round bottom flask. To this solution, TEA (894 μL, 6.45 mmol) was added and the solution was stirred for 5 min. 4-pentylbenzoyl chloride (290 μL, 1.42 mmol) was then added dropwise to reaction and stirred at ambient temperature for 2 hr, then at 135 °C for 22 hr. The round bottom flask was cooled to room temperature, rinsed with EtOAc (20 mL) and H₂O (15 mL). The organic layer was extracted, dried over Na₂SO₄, filtered, and concentrated to dryness. The crude oil was then purified via flash column chromatography using 5:1 Hex/EtOAc to 3:1 Hex/EtOAc to give a colorless oil (212.0 mg, 76% yield). ¹H NMR (300 MHz, CDCl₃), δ 7.84 (d, J = 8.4 Hz, 2H), 7.20 (d, J = 8.1 Hz, 2H), 4.43-4.36 (m, 2H), 4.06-3.99 (m, 2H), 2.62 (t, J = 7.5 Hz, 2H), 1.63-1.58 (m, 2H), 1.32-1.27 (m, 4H), 0.87 (t, J = 6.9 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃), δ 164.8, 146.7, 129.8, 128.7, 128.3, 127.1, 125.2, 67.6, 55.0, 35.9, 31.5, 31.0, 22.6, 14.1; HRMS (ESI) calcd. for C₁₄H₁₉NO [M+H]⁺: 218.15394, found: 218.15378.
Representative NMR spectra.
Pulse Sequence: s2pu1
Solvent: CCl3
Ambient temperature: Mercury-3000B
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acc. time 1.975 sec
Vista 4508 Hz
16 repetitions
Field strength 399.7915 MHz
DATA PROCESSING
FT 6124 32768
Total time 3 min, 18 sec
Pulse Sequence: s2pol
Solvent: CDCl3
Ambient temperature
Mercury-400B  "acmeac-400"
Polar 26.0 degrees
Avg. time 1.160 sec
Width 20800.0 Hz
4418 repetitions
Observer, 414.6119817 MHz
Observer, 414.6119827 MHz
Power 46 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65520
Total time 3 hr, 34 min, 55 sec
Pulse Sequence: zspul
Solvent: CDC12
Ambient Temperature: Mercury-300MB "oven temperature" 300C
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.005 sec
16 repetition
OBERON NS 399.918181 MHz
DATA PROCESSING
f1 slice 32768
Total time 0 min, 45 sec
**Pulse Sequence:** eapw1

- **Solvent:** CDCl3
- **Ambient temperature:** 300 K (27°C)
- **Relax. delay:** 1.0 sec
- **Pulse:** 90°
- **Acq. time:** 1.0 sec
- **Width:** 509.5 Hz
- **10 repetitions
- **Data Processing:**
  - **FT size:** 32768
  - **Total time:** 9 min, 43 sec
Pulse Sequence: sdpul
Solvent: CDCl3
Ambient temperature
Mercury-400B "VGSsmerg02"

Pulse 28.8 degrees
Arg. time 0.150 sec
Width 50000 Hz
T1 3000 sec
R1 600000 Hz
R2 10000 Hz
OBSERVE 613.100000 MHz
DECOUPL e 600.116000 MHz
Power 48 dB
Continuously on
WALTZ-15 decoupled
DATA PROCESSING

FT size 9532X16
Total time 3 hr, 9 min, 47 sec
References


